

# PERCOLATION TRANSITION IN THE RANDOM ANTIFERROMAGNETIC SPIN-1 CHAIN

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## Abstract

We give a physical description in terms of percolation theory of the phase transition that occurs when the disorder increases in the random antiferromagnetic spin-1 chain between a gapless phase with topological order and a random singlet phase. We study the statistical properties of the percolation clusters by numerical simulations, and we compute exact exponents characterizing the transition by a real-space renormalization group calculation.

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Antiferromagnetic quantum spin chains are known to present vastly different physical properties according to whether the spin value is integer or half-integer [1]. In the case of integer spin, there is a (Haldane) gap for magnetic excitations and short-range magnetic order. In the case of half-integer spin, there is quasi-long range spin order with algebraically decaying spin correlations and no gap. An appealing physical picture of the integer-spin case is given by the so-called valence-bond-solid (VBS) wavefunctions [2]. With these approximate ground states, it is easy to see that there is a hidden long-range order that is non-local in terms of the true spins-1 [3]. These properties are well established for the pure systems but it is obviously important to understand what happens in the disordered case. Bond disorder in a quantum spin chain may be realized experimentally by chemical substitution of the ligand that induces superexchange between the spins, for example. This leads to a Heisenberg Hamiltonian:

$$H = \sum_i J_i \vec{S}_i \cdot \vec{S}_{i+1}, \quad (1)$$

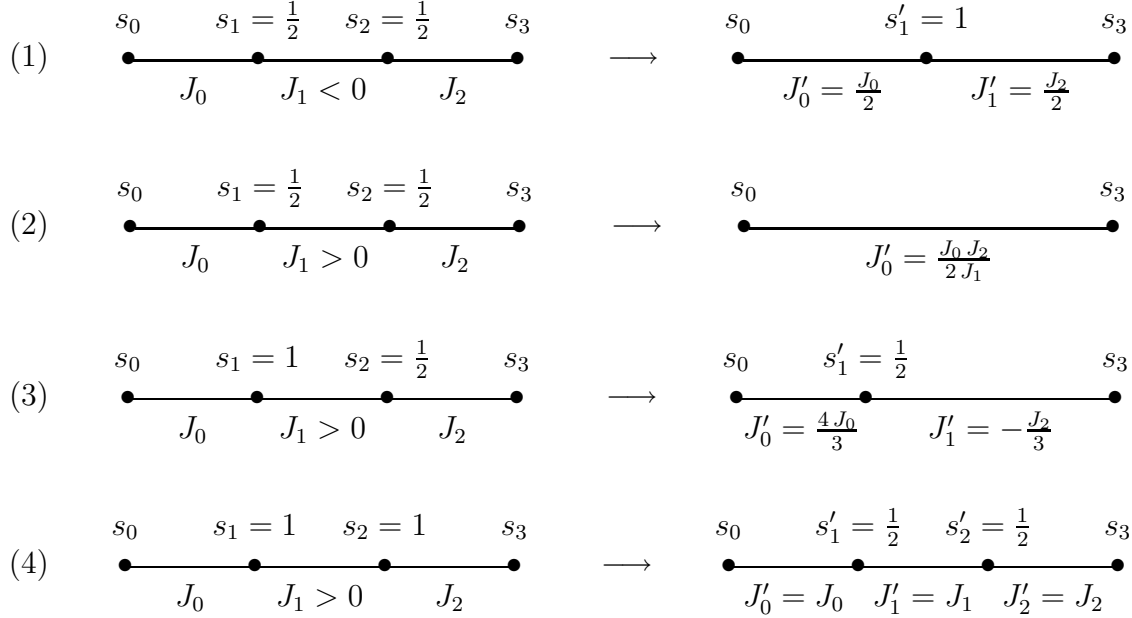
where  $\vec{S}_i$  are quantum spin operators and the couplings  $J_i$  are quenched random variables. In the spin-1/2 case, it is known [4,5] that for any strength of the disorder the system goes to the so-called random singlet phase [6] in which the spins are paired into singlets over arbitrarily large distances. The effect of randomness on other quantum spin chains has also been investigated recently [7–11].

In the spin-1 case, it has been shown [12,13] that this random singlet phase appears only when the randomness is strong enough. These results have been obtained by an asymptotically exact real-space renormalization group (RG) study on an effective spin-1/2 model. For weak disorder, there is a phase which is gapless but sustains hidden long-range order. This is analogous to gapless superconductivity that occurs when doping a superconductor with magnetic impurities; here the role of the superconducting condensate is played by the hidden order.

In this Letter, we use a real-space renormalization procedure that leads to an appealing percolation picture of the phase transition that occurs in the disordered antiferromagnetic spin-1 chain. We formulate the hidden long-range order in terms of a macroscopic VBS-cluster. This allows us to define several critical exponents to describe this phase transition. We study them by direct numerical renormalization and compare to the exact values that we obtain for the effective model of Ref. [12] which is in the same universality class.

An efficient technique to study random spin chains is the real-space renormalization group [4,5]. The basic idea is to integrate out the strongest bond of the chain and to compute in perturbation theory the corresponding renormalization of the coupling strengths distribution. This can be done iteratively and, in the case of the  $S=1/2$  chain, leads to a universal fixed point distribution which is extremely broad, the so-called random singlet phase [4]. However, when generalized to higher spin values, this method is blind to the difference between integer and half-integer spins. To capture the physics of the Haldane phase of the random spin-1 chain, we need to introduce an extended set of spin chains described by the Hamiltonian (1), where  $\vec{S}_i$  is a spin-operator of size  $s_i = 1/2$  or  $s_i = 1$ , and where the couplings  $\{J_i\}$  can be either ferromagnetic (F) or antiferromagnetic (F), but have to satisfy the following constraint : for any chain segment  $\{i, j\}$ , the classical magnetization must satisfy  $|m_{i,j}| \leq 1$ .

This condition for  $j = i+1$  implies that there are four types of bonds : i) F bond between two spins  $S=1/2$ , ii) AF bond between two spins  $S=1/2$ , iii) AF bond between one spin  $S=1$  and one spin  $S=1/2$ , iv) AF bond between two spins  $S=1$ . The decimation procedure is the following : to each bond ( $i$ ), we associate the energy difference  $\Delta_i$  between the highest state and the lowest state of the Hamiltonian  $J_i \vec{S}_i \cdot \vec{S}_{i+1}$ . We pick up the bond  $(\vec{S}_i, \vec{S}_{i+1}, J_i)$  corresponding to the strongest  $\Delta_i$  of the chain. To define the renormalization rule for this bond, we divide the four-spin Hamiltonian into  $H_i = h_0 + h_1$  where  $h_0 = J_i \vec{S}_i \cdot \vec{S}_{i+1}$  and  $h_1 = J_{i-1} \vec{S}_{i-1} \cdot \vec{S}_i + J_{i+1} \vec{S}_{i+1} \cdot \vec{S}_{i+2}$ . We treat  $h_1$  as a perturbation of  $h_0$  to find the effective Hamiltonian replacing  $H_i$  when the highest energy state of  $h_0$  is removed. This leads to the four following renormalizations rules:



These rules are a slight modification of those proposed by Hyman [13]. Our renormalization procedure is entirely consistent from the point of view of the progressive elimination of the highest energy degrees of freedom : all the energy scales of the new bonds are always smaller than the energy scale of the old bond. It is also easy to check that this procedure is “closed” inside the enlarged set of spin-chains defined above. In particular, spins higher than 1 cannot appear in this scheme [14].

If we represent each spin-1 as the symmetrization of two spin-1/2, the rules 2, 3, and 4 for AF bonds may then be interpreted as the formation of a singlet between two constitutive spin-1/2. The rule 1 for a F bond between two spin-1/2 corresponds to their symmetrization. As a consequence, at the end of the renormalization procedure, when there are no free spins left, the chain decomposes itself into a set of disconnected clusters that have the structure of a VBS-state (see Figure 1). The topological order can be probed by use of the string order parameter [3] defined as:

$$t_{ij} = -\langle \psi_0 | S_i^z \exp \left[ i\pi \sum_{i < k < j} S_k^z \right] S_j^z | \psi_0 \rangle. \quad (2)$$

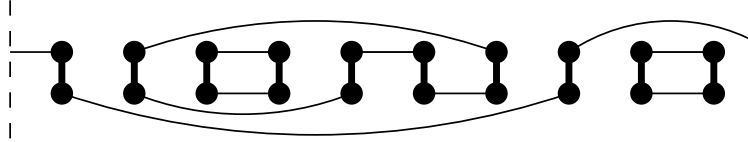


FIG. 1. The ground state of the random chain obtained from the real-space renormalization. Each spin  $S=1$  is written as two symmetrized spins  $S=1/2$ : the black dots related by a vertical thick line. Spins are grouped in clusters related by singlet bonds that are the thin lines. There are two clusters of size 2, one of size 4, and one larger cluster that extends beyond the limits of the figure.

For the pure VBS state on a finite ring of  $n$  spins  $S=1$ , one has  $t_{ij} = 4/9$  (up to corrections of  $O(3^{-n})$  that we neglect in the following). Now for the disordered system, one has  $t_{ij} = 4/9$  if the two sites do belong to the same cluster and  $t_{ij} = 0$  if they don't. We thus consider, for a given realization of the disorder on a chain of  $N$  spins, the spatial average of the string order parameter  $\sum_{i,j} t_{ij}/N^2$  which is equal to  $4/9 \times T$  where:

$$T \equiv \sum_c \frac{n_c^2}{N^2} = \frac{9}{4} \frac{1}{N^2} \sum_{i,j} t_{ij} + O(1/N). \quad (3)$$

Here  $c$  is the cluster index and  $n_c$  is the number of spins of the cluster, i.e. its size (which is not directly related to its spatial extent). This quantity  $T$  is the probability that two randomly chosen spins belong to the same cluster. It is also the mean size of the cluster containing a randomly chosen spin, divided by  $N$ . This order parameter can be non-zero in the large- $N$  limit only if at least one VBS-cluster contains a finite fraction of the spins of the chain.

We have simulated the renormalization procedure on spin-1 chains containing  $N$  sites with periodic boundary conditions. The initial couplings  $J_i$  are uniformly distributed in the interval  $[1, 1 + d]$ . The parameter  $d$  measures the strength of the initial disorder. We have numerically implemented the renormalization rules on  $M$  initial independent samples, and averaged quantities over these different realizations of the disorder. Typically the averaging process has been performed on  $N \times M \approx 10^9$  spins. The plot of  $T$  as a function of the disorder for various sizes in Figure 2 shows clearly that the phenomenology for the clusters is similar to the physics of percolation. Indeed we observe a small-disorder phase in which there is exactly one macroscopic cluster ( $c=1$ ) that contains a nonzero fraction  $n_1/N$  of the spins in the thermodynamic limit. There is also a distribution of finite clusters, i.e. non-diverging with  $N$ . This phase with  $T \neq 0$  has long-range hidden order. There is a critical value  $d_c$  of the disorder for which the diverging cluster disappears, i.e.  $T$  vanishes. Then, for larger randomness  $d > d_c$ , there are only finite clusters and  $T = 0$ .

Following the notations of percolation theory [15], we denote by  $\beta$  the exponent describing the vanishing of the fraction  $n_1/N$  of spins in the macroscopic cluster. The order parameter thus scales as  $T \sim (d_c - d)^{2\beta}$  for  $d < d_c$ . The finite size scaling study of Fig. 2 leads to the following estimate:

$$2\beta = 1.0(1). \quad (4)$$

On Figure 3, we have plotted the mean size of finite clusters, which plays the role of the

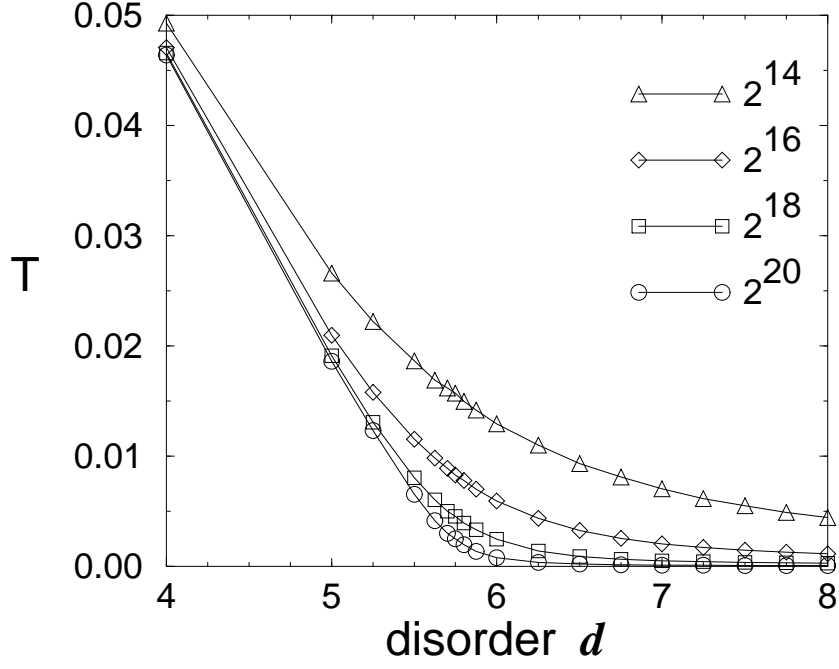


FIG. 2. String order parameter  $T$  as a function of the disorder  $d$  for sizes  $N = 2^{14} - 2^{20}$ . The critical point is  $d_c = 5.76(2)$

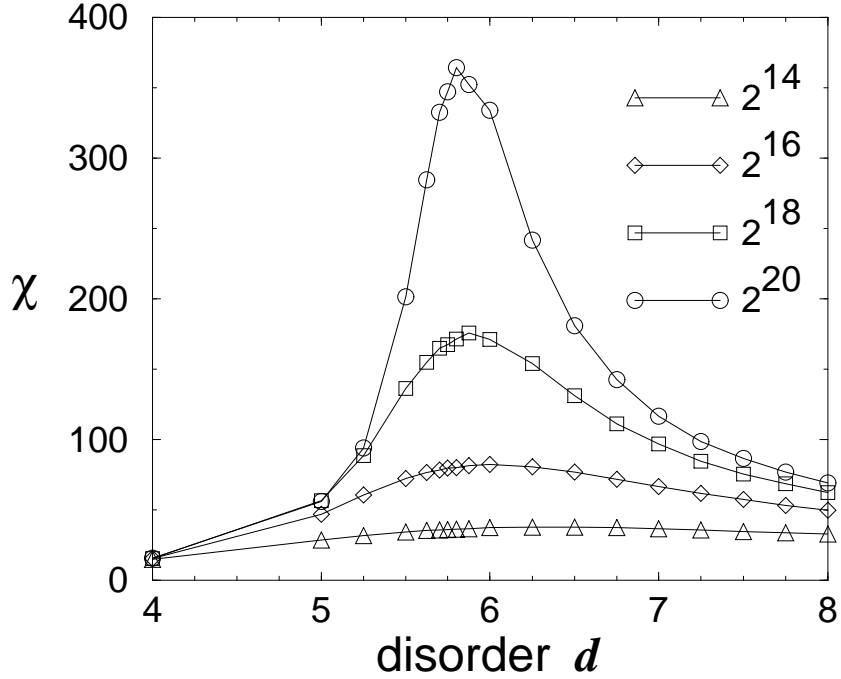


FIG. 3. Percolation susceptibility  $\chi$ , i.e. mean size of finite clusters, as a function of disorder, for sizes  $N = 2^{14} - 2^{20}$ .

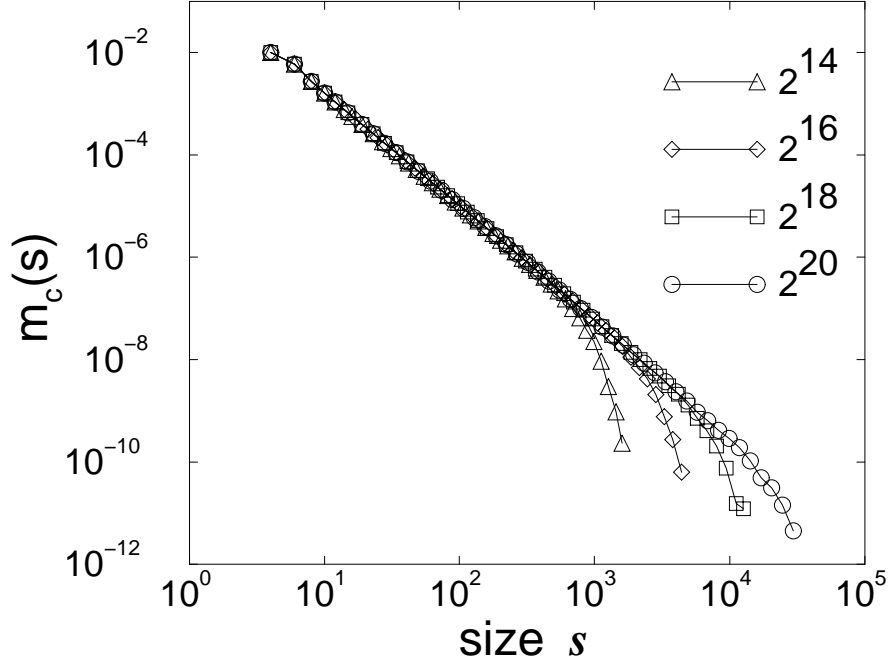


FIG. 4. Cluster size distribution  $m_c(s)$  as a function of size  $s$ , at criticality. The slope leads to  $\tau = 2.2(1)$ .

percolation susceptibility:

$$\chi \equiv \sum_{c>1} \frac{n_c^2}{N}. \quad (5)$$

In the sum, note that we omit the biggest cluster ( $c=1$ ). Denoting by  $\gamma$  the exponent describing the divergence of this quantity,  $\chi \sim |d_c - d|^{-\gamma}$ , we have performed a finite size scaling study which leads to the value :

$$\gamma = 1.2(1). \quad (6)$$

Let us call  $m_d(s)$  the number of clusters of size  $s$ , divided by  $N$ . Then standard scaling leads to the formula valid in the limit  $N \rightarrow \infty$  [15] :

$$m_d(s) \sim \frac{1}{s^\tau} f[(d_c - d)s^\sigma] \quad (7)$$

where  $f(z)$  is a scaling function. The exponent  $\sigma$  defines the divergence of the characteristic cluster size as  $|d_c - d|^{-1/\sigma}$  and the exponent  $\tau$  characterizes the algebraic decay of the distribution of cluster sizes at the critical disorder  $d_c$ . These exponents can be related to  $\beta$  and  $\gamma$  as in percolation theory according to  $\beta = (\tau - 2)/\sigma$  and  $\gamma = (3 - \tau)/\sigma$ . In Fig. 4, we have plotted the distribution of cluster sizes at criticality  $d = d_c$ . Measurement of the slope leads to the following estimate of the exponent  $\tau$ :

$$\tau = 2.2(1). \quad (8)$$

We now show that the exponents that appear naturally in the percolation picture can be obtained exactly. First, we explain how the VBS-clusters appear in the random dimerized spin-1/2 chain model of Hyman and Yang [12], which is an effective model for the random AF spin-1 chain. We briefly recall the properties of the effective model that are necessary for our purposes. In this model, all even bonds are AF, whereas the odd bonds are either F or AF. At any stage of their renormalization procedure, the energy scale  $\Omega$  is given by the strongest AF bond of the system, so that the odd bonds separate into two groups : group A contains all AF bonds and F bonds weaker than  $\Omega$ , while group B contains all F bonds stronger than  $\Omega$ . In this effective model, perfect VBS order means singlets over all even bonds of the initial chain. Indeed, at the stable fixed point of the Haldane phase found in [12] by solving the renormalization flow equations, all odd bonds are much weaker than even bonds so that only singlets over even bonds are generated by decimation. It is convenient to introduce in their procedure an auxiliary variable  $\mu$  for each odd bond still surviving at scale  $\Omega$ . The variable  $\mu$  is by definition the number of singlets already made over even bonds of the initial chain that are contained in this odd bond. The evolution rules for this new variable are the following : when an odd bond of variable ( $\mu$ ) is decimated, a finite cluster of size ( $\mu + 1$ ) is terminated; when an even bond surrounded by two odd bonds of group B of variables  $\mu_1$  and  $\mu_2$  respectively, a finite cluster of size ( $\mu_1 + \mu_2 + 2$ ) is terminated; when an even bond surrounded by two odd bonds of group A, or surrounded by one odd bond of group A or one odd bond of group B, with respective variables  $\mu_1$  and  $\mu_2$ , the new odd bond generated by this decimation inherits the variable ( $\mu = \mu_1 + \mu_2 + 1$ ). Following the method outlined by Fisher [5], we find that, at the fixed point describing the transition of the effective model, the auxiliary variable  $\mu$  scales with  $\Gamma = \ln(\Omega_0/\Omega)$  (where  $\Omega_0$  is the initial cut-off) as :

$$\mu \propto \Gamma^\varphi \quad \text{with } \varphi = \sqrt{5}. \quad (9)$$

This has to be compared with the scaling  $l \propto \Gamma^3$  of the auxiliary variable  $l$  that counts the number of initial bonds in a surviving bond at scale  $\Gamma$ . Deviations from the critical point are driven by a relevant perturbation [12] that scales as  $\Gamma^{\lambda_+}$  with  $\lambda_+ = (\sqrt{13} - 1)/2$ . As a consequence, the exact exponent for the string topological order parameter (4) is [16] :

$$2\beta = \frac{2(3 - \varphi)}{\lambda_+} = \frac{4(3 - \sqrt{5})}{\sqrt{13} - 1} = 1.17278..., \quad (10)$$

the exponent of the percolation susceptibility is :

$$\gamma = \frac{(2\varphi - 3)}{\lambda_+} = \frac{2(2\sqrt{5} - 3)}{\sqrt{13} - 1} = 1.13000..., \quad (11)$$

and the exponent  $\tau$  of the scaling form (7) for the distribution of cluster sizes :

$$\tau = 1 + \frac{3}{\varphi} = 1 + \frac{3}{\sqrt{5}} = 2.34164..., \quad (12)$$

in agreement with our numerical estimates (4), (6), (8).

In this Letter, we have given a percolation picture of the random spin-1 chain. Topological long-range order characteristic of the Haldane phase is due to the existence of a single cluster of spins related in a VBS manner whose size diverges in the thermodynamic limit. The transition to the random singlet phase with increasing disorder leads to the vanishing of the string order parameter with an exponent  $2\beta = 1.17$  while the percolation susceptibility diverges with an exponent  $\gamma = 1.13$ . These exponents are exact because the RG procedure is asymptotically exact [5].

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- [16] The correct definition of the VBS clusters implies that the variable  $\mu$  differs from the definition of active spins introduced in [12]. Our scaling exponent  $\varphi$  differs from the exponent  $\phi = 2$  of active spins. The exponent  $2\beta$  is not equal to the value  $2/\lambda_+ = 1.53518\dots$  found in [12].